

Spectroscopy of ultracold atoms by periodic lattice modulations

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We present a non-perturbative analysis of a new experimental technique for probing ultracold bosons in an optical lattice by periodic lattice depth modulations. This is done using the time-dependent density-matrix renormalization group method. We find that sharp energy absorption peaks are not unique to the Mott insulating phase at commensurate filling, but also exist for superfluids at incommensurate filling. For strong interactions the peak structure provides an experimental measure of the interaction strength. Moreover, the peak height of the peaks at $\hbar\omega \gtrsim 2U$ can be employed as a measure of the incommensurability of the system.

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The experimental realization of Bose-Einstein condensation in weakly interacting ultracold atoms opened the way to numerous exciting experiments directly probing fundamental effects of quantum mechanics. More recently, the regime of strongly interacting atoms has become experimentally accessible by Feshbach resonances [1] and the advent of ultracold atoms in optical lattices [2, 3]. In a pioneering experiment, the quantum phase transition from a bosonic Mott insulator to a superfluid has been demonstrated [3]. More generally, ultracold atoms in optical lattices open up the possibility to simulate and explore complex quantum many-body phenomena known from electronic solids, like high-temperature superconductivity, in a new context [4]. One major advantage of ultracold atom systems compared to their condensed matter counterparts is the tunability of the system parameters. In particular, fast tunability in time made a whole area of new non-equilibrium phenomena experimentally accessible [3, 5, 6]. The theoretical description of these phenomena, especially beyond linear response, is still lacking. To probe quantum states in cold atoms, various new measurement techniques have been developed. Light-induced Bragg scattering yields the dynamical structure factor [7], while RF absorption provides information about single-particle excitations [8]. Time-of-flight expansion gives access to the momentum distribution and correlations via detection of the average density and noise [9]. Nevertheless, there is still a lack of measurement techniques compared to condensed matter setups.

A qualitatively new way of probing the system which exploits fast tunability was introduced by Stöferle *et al.* [6]. They determined the excitation spectrum of ultracold bosons in an optical lattice by measuring the heating induced by a relatively strong periodical modulation of the lattice height (20% of the initial lattice height). Three distinct peaks at different frequencies were observed in the energy absorption. Up to now, these features, in particular the second and the third peak, are not well understood. Previous theoretical studies applied

a linear response treatment [10, 11, 12, 13] in analogy to condensed matter systems or considered weak interactions using the Gross-Pitaevskii equation [14]. However, the relatively strong modulation and the presence of a trapping potential in the experiments, which implies inhomogeneous filling [15, 16], demand for alternative methods to check the validity of previous approximations.

In this Letter we present what is to our knowledge the first simulation of the experiment by Stöferle *et al.* taking the full time-dependence into account for reasonable system sizes in the regime of strong and intermediate interaction. Hereby, we focus on one spatial dimension using the adaptive time-dependent density-matrix renormalization group method (adaptive t-DMRG) [17, 18]. It is a numerical method that allows for real-time evolution of quantum many-body systems out of equilibrium with an explicitly time-dependent Hamiltonian. For the case of commensurate filling we compare for weak modulations our results to the analytical results of Iucci *et al.* [10] to show the reliability of our method. For large modulations saturation effects occur and reduce the height of the absorption peaks. We show that at low temperature incommensurate regions with more than one particle per site are crucial to reproduce the multiple peak structure of the experimental absorption spectrum. The appearance of the peak structure is not a specific sign of the Mott insulating state as widely believed, but reflects the gap occurring for strong repulsion between the coupled energy bands (Hubbard bands). For strong interactions the peak positions can be used as an experimental measure of the interaction strength. We also show that the height of the peak at frequencies $\hbar\omega \gtrsim 2U$ can be employed as a measure of the incommensurability of the system. Such a measure is highly relevant for the realization of quantum computing with ultracold atoms in optical lattices, since for current proposals the formation of wide regions with commensurate filling is crucial.

The Bose-Hubbard model [15, 19]

$$H = -J \sum_{j=1}^{L-1} (b_j^\dagger b_{j+1} + h.c.) + \frac{U}{2} \sum_{j=1}^L \hat{n}_j(\hat{n}_j - 1) + \sum_{j=1}^L \varepsilon_j \hat{n}_j,$$

describes well ultracold bosons in a one-dimensional system subjected to an optical lattice. Here L is the number of sites in the chain, b_j^\dagger and b_j are the creation and annihilation operators, and $\hat{n}_j = b_j^\dagger b_j$ is the number operator on site j . The parameters J and U are the hopping amplitude and the onsite interaction strength. The third term models the chemical potential or an external potential, like the trapping potential. In a system with commensurate filling a quantum phase transition occurs at a finite ratio $(U/J)_c$ between a Mott insulating phase, in which the atoms are strongly localized at the lattice sites, and a superfluid phase with delocalized atoms. For incommensurate filling, however, it is energetically unfavorable to localize all the atoms and the system remains superfluid. The parameters of the Bose-Hubbard model are directly related to experimental quantities. For large lattice sizes an approximate formula is given by [20] $J/E_r = (4/\sqrt{\pi})(V_x/E_r)^{(3/4)} \exp(-2\sqrt{V_x/E_r})$ and $U/E_r = 4\sqrt{2\pi}(a_s/\lambda)(V_x V_\perp^2/E_r^3)^{(1/4)}$. Here E_r is the recoil energy, a_s is the s -wave scattering length, and λ is the wavelength of the laser of the optical lattice. V_x denotes the height of the optical lattice and V_\perp the strongly confined transverse direction [24]. For a better comparison to the experiment [6] we use $a_s = 5.45\text{nm}$ of ^{87}Rb in the $F = 2$, $m_F = 2$ hyperfine state and $\lambda = 825\text{nm}$. A periodical modulation of the lattice height, here we use $V_x(t) = V_0[1 + \delta V \cos(\omega t)]$, translates into a periodic variation of the hopping coefficient J and the interaction coefficient U via $J(t) = J[V_x(t)]$ and $U(t) = U[V_x(t)]$.

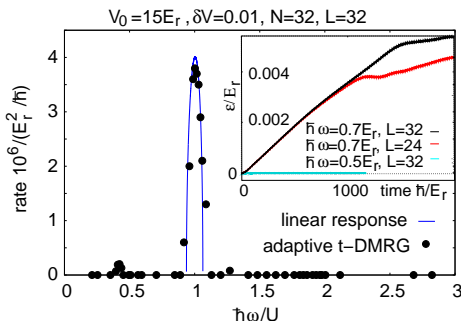


FIG. 1: Absorption rate vs. the modulation frequency ω at a lattice depth $V_0 = 15E_r$; the corresponding values of the Bose-Hubbard model are $U \approx 0.71E_r$ and $J \approx 0.0074E_r$, i.e. $U/J \approx 95$. The lines are analytical results obtained by linear response treating the hopping term as a perturbation [10]. The symbols are the results obtained using the adaptive t-DMRG. Inset: Energy absorbed versus time. $\omega = 0.71E_r/\hbar$ corresponds to a modulation frequency at resonance and $\omega = 0.5E_r/\hbar$ away of resonance.

In Fig. 1 the dependence of the energy absorption rate on the modulation frequency is shown for a system which is initially in the Mott insulating phase with filling $n = 1$ per lattice site [25]. We found this rate α to be independent of the system size before saturation occurs (see inset Fig. 1). It is determined by fitting the function $f(t) = E(t=0) + \alpha t + b_1 \cos(\omega t + b_2)$ with the fitting parameters α , b_1 , and b_2 to our results before saturation. The rate shows a two peak structure: a large peak at $\hbar\omega \approx U$ and an approximately 20 times smaller one at $\hbar\omega \approx U/2$. The peak at $\hbar\omega \approx U$, in the following called U peak, corresponds to particle-hole excitations by a “single photon” process [6, 10, 11, 12]. For a small modulation amplitude $\delta V = 0.01$ the results for the U peak obtained by linear response combined with perturbation theory in J/U (solid lines) agree very well with our full calculation. The peak at $\hbar\omega \approx U/2$, which does not occur in linear response, is due to “two-photon” processes where twice the energy quantum is needed to generate a particle-hole excitation [21]. In principle absorption peaks at frequencies which are higher multiples of U can also arise. For commensurate filling, our calculations demonstrate that they are negligible [26].

Up to now we considered an initially Mott insulating state. However, if the filling is incommensurate, the system remains superfluid for all interaction strengths. In the limit of strong interaction, energy bands (Hubbard bands) occur separated by an energy gap of order U , but the system remains superfluid, since excitations in the highest occupied band are gapless. Therefore, as pointed out before [10, 12, 14], incommensurability changes the low ($\omega \ll U/\hbar$) frequency spectrum. However, the presence of a trap and the experimental resolution makes it difficult to observe this change in experiment. We show how incommensurability also imprints clear signatures in the high ($\omega \sim 2U/\hbar$) frequency spectrum.

For a deep lattice, see Fig. 2 (a), in addition to the U peak a new resonance at $\hbar\omega \approx 2U$, in the following called $2U$ peak, arises [27]. The main contribution to it stems from the process in which one particle hops onto an already doubly occupied site. The process where two particle-hole excitations are created is negligible. Therefore the $2U$ peak is a clear indicator for regions of the optical lattice with incommensurate filling. For the homogeneous system considered here we find that even at zero temperature the $2U$ peak for an incommensurate filling $n \approx 1.2$ is much higher than the U peak. Finite temperature could generate further defects in the occupation and thereby additional contributions to the $2U$ peak as noted in [11] for the commensurate system [28]. The peak height of the $2U$ peak could be taken as a measure of the ‘degree’ of incommensurability present in the system regardless of the origin of the incommensurability. The same finding holds for larger values of the hopping parameter. The peak structure becomes more complicated [cf. Fig. 2 (b)], but the peaks at $\hbar\omega \approx 2U$ and

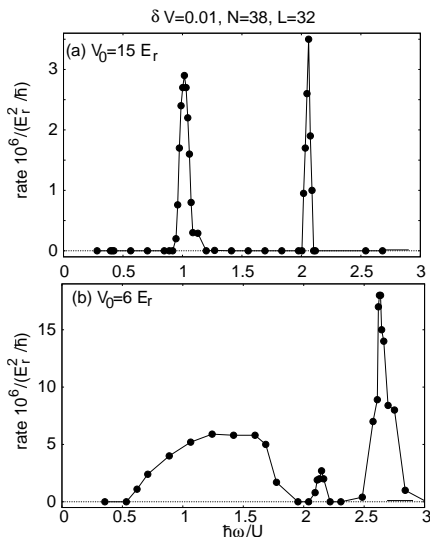


FIG. 2: Energy absorption rate vs. modulation frequency ω at incommensurate filling $N = 38$ particles on $L = 32$ sites for a lattice height of (a) $V_0 = 15E_r$ and (b) $V_0 = 6E_r$. Compared to the system at commensurate filling additional peaks at $\hbar\omega \approx 2U$ and in (b) at $\hbar\omega \approx 2.6U$ arise. Solid lines are guide to the eyes.

$\hbar\omega \approx 2.6U$ still only appear for incommensurably filled systems. The shift in position compared to the naively expected positions at integer multiples of U can be understood from the change in the energy structure. Whereas for strong interactions narrow energy bands with a gap of U exist, for intermediate interactions the bands broaden with increasing hopping. In particular, the ground state of the incommensurate system shifts down strongly with increasing hopping strength. As a result, the energy difference towards excited states increases which causes in Fig. 2 (b) the shift of the center of the U peak to approximately $1.2U$ and of the $2U$ peak to approximately $2.6U$. The peak around $2.1U$ stems from a splitting of the U band in processes in which a particle hole pair is created on singly occupied sites and doubly occupied sites. The ratio of the amplitudes of the peaks depends crucially on the degree of incommensurability in the system. We have verified these findings by exact diagonalization of Bose-Hubbard chains up to 7 sites.

In order to use this $2U$ peak as a measure of the amount of incommensurability, one needs to determine it for the strong modulations ($\sim 20\%$) used in the existing experiments [6]. The adaptive t-DMRG method, which has no problem dealing with the strong time dependent modulation, is thus ideally suited to tackle this question whereas it is delicate to use linear response for this purpose. To illustrate the difference we compare in Fig. 3 the energy absorption rate for the case of a small modulation $\delta V_1 = 0.01$ and a modulation with the strength $\delta V_2 = 0.2$. The results for δV_1 are rescaled by a factor of

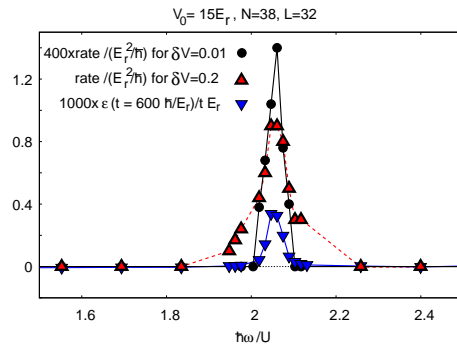


FIG. 3: Saturation effects for strong modulations. The absorption rate for a weak modulation (a) $\delta V_1 = 0.01$ (circles) and a strong modulation (b) $\delta V_2 = 0.2$ (upward triangles) are compared. The rate for (a) is scaled by the ratio $(\delta V_2/\delta V_1)^2$ to remove trivial scaling. Clear saturation effects in the peak height and width can be seen. Saturation of the integrated energy absorption in time: (c) is the integrated energy absorbed up to time $t_m = 600\hbar/E_r$ per unit time (downward triangles), i.e. $[E(t_m) - E(0)]/t_m$ for $\delta V_2 = 0.2$. The chosen value of $\delta V_2 = 0.2$ and $t_m = 600\hbar/E_r$ correspond to the experimental values. Due to saturation effects in time it is smaller than the energy absorption rate shown in (a).

$(\delta V_2/\delta V_1)^2$ to eliminate the trivial amplitude dependence expected from linear response. Although the structure of center of the peak agree qualitatively well even for these high modulation strength, saturation effects occur in particular in the height of the peaks. Our results indicate that linear response overestimates the actual energy absorption. For the parameters shown here a reduction by a factor of approximately 1.6 takes place. A bimodal structure seems to appear for strong modulations which causes a broadening of the peaks, here by a factor of approximately 2. We also plotted the experimentally measured quantity, namely the heating, i.e. the integrated absorbed energy. In Fig. 3 we show $[E(t_m) - E(0)]/t_m$ for a modulation time $t_m = 600\hbar/E_r$ chosen as in the experiment. The positions of the peaks agree well in the two spectra but the height deviates, for the parameter shown here approximately by a factor of 2. This is mainly due to saturation effects in time (cf. inset Fig. 1) which cause the actual integrated absorption per unit time to remain lower than the rate [29].

In order to relate our results to present day experiments we have to investigate how much the trap affects the energy absorption spectrum. We find that the positions of the peaks are robust against the presence of a trapping potential [30] and that the amplitudes remain of the same order of magnitude. This findings can be seen in Fig. 4 in which we show an example of the integrated absorbed energy at a fixed time t_m versus the modulation frequency for the case of the presence of an incommensurate region in the center of the parabolic trap (see inset Fig. 4)[31]. Therefore as in the homogeneous

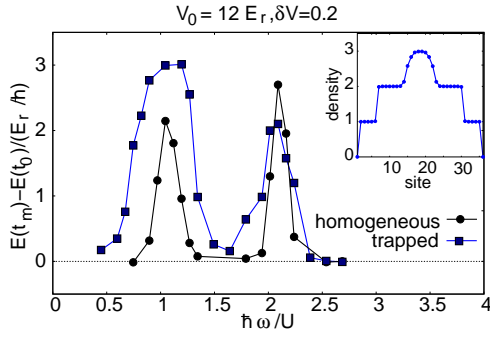


FIG. 4: The integrated energy absorbed up to time $t_m = 50\hbar/E_r$, i.e. $[E(t_m) - E(0)]$ for $\delta V_2 = 0.2$ in a system with confining potential and $N=65$ (squares) and in a homogeneous system with $N=46$ and $L=32$ (circles). The inset shows the initial density distribution in the trapped system.

case the occurrence of a peak at $\hbar\omega \approx 2U$ signals the presence of an incommensurate region and our findings enables us to compare the positions in the homogeneous system (Fig. 2) to the experimental data [6].

In the experiment for large values of the initial lattice height narrow peaks at $\hbar\omega \approx U$ and $\hbar\omega \approx 2U$ were found. These peaks broaden and shift in energy if the lattice becomes more shallow. For intermediate interaction strength an additional peak at $\hbar\omega \approx 2.6U$ appeared. These findings for the positions of the peaks agree excellently with our results at zero temperature *provided* we assume the presence of an incommensurately filled region in the experimental system (cf. Fig. 2).

To conclude we have demonstrated using the adaptive t-DMRG method that the measurement procedure [6] gives important information about the properties of the bosonic system, in particular about commensurability properties and the energy levels. It will therefore be of great interest to extend these calculations and measurements to cold fermions in optical lattices, which have only recently been realized experimentally [22].

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- [24] Here we use the tight transverse confinement $V_{\perp} \equiv 30E_r$.
- [25] In our adaptive t-DMRG calculation the explicit time-dependence of the Hamiltonian was approximated by a sequence of small time steps with time-independent Hamiltonians. Step sizes (down to $0.2\hbar/E_r$) were determined by a convergence analysis. We keep several hundred states in the effective Hilbert space (see Ref. [23] for a detailed error analysis).
- [26] This can also be understood from a perturbative calculation: to first order only the U peak has non-vanishing weight in a commensurately filled system; the linear response matrix elements at $2U$ vanish as $(J/U)^3$. The $3U$ peak results from two contributions: i) three particle-hole excitations, and ii) two particle hole excitations with both particles jumping on the same site. The matrix element of the process i) vanishes faster than J/U and therefore only the process ii) contributes to the $3U$ peak at this order.
- [27] The peak at $\hbar\omega \approx U/2$ is much smaller and cannot be seen here. The height of the peak at $\hbar\omega \approx U$ decreases compared to the commensurate case (cf. Fig. 2 and 1).
- [28] In a commensurate system a high temperature of $T = U/3$ is necessary to generate a second peak of considerable height [11]. This temperature is much higher than the one expected in the experimental setup.
- [29] In contrast the width of the absorption peaks is smaller than the width found for the rate with the same modulation strength (20%) and resembles the width found

for the rate of a smaller modulation strength (1%). A detailed study of the saturation effects goes beyond the scope of the work presented here.

- [30] This is expected by the simple picture in which particle hole excitations are created on neighbouring sites. There the trapping only causes a shift of the excitation energy by the difference of the site on which the particle hole pair is generated. Since the sign of the shift depends on which site the particle and on which the hole is created it will lead to a simple broadening.
- [31] We used a potential of the form $V_t = 0.006(j - L/2 -$

$1/2)^2$. The results for the initial state may have large uncertainties at the boundaries of locked phases, since here many states almost degenerate in energy exist. Nevertheless, this should not change the qualitative picture found. Due to computational reasons the time t_m is chosen smaller than in the experiment. We found that by this we underestimate the amplitude of the $2U$ peak compared to the U peak compared to the experiment, since it grows with time t_m .